Thermophoretic accumulation in hydrothermal pores

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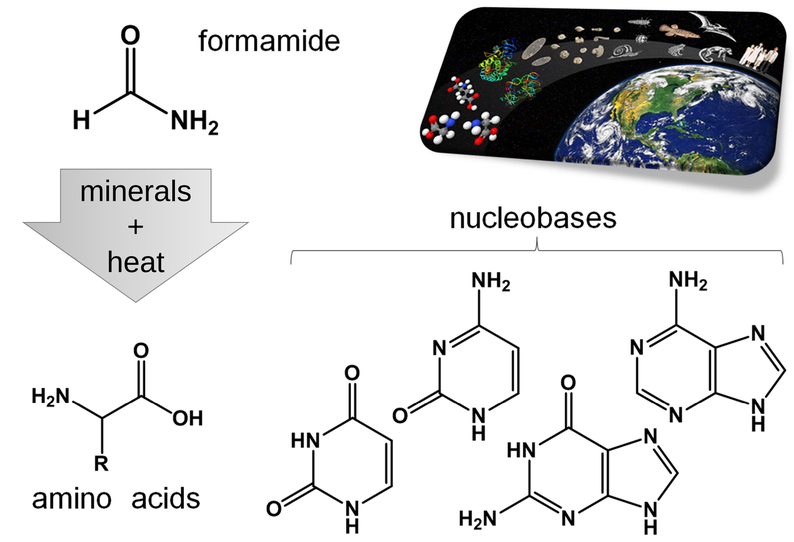
Introduction

Formamide has been shown to form prebiotic molecules under catalytic conditions.[1] These findings assume a high formamide concentration. On early earth this would only be possible through accumulation.[2] The thermophoretic behaviour of the formamide/water system was measured. Finite element simulations show that a high degree of formamide accumulation in hydrothermal pores is possible.[3]

[1] R. Saladino *et al.*, *Physics of Life Reviews* **9** (2012) 84
[2] S. Miyakawa *et al.*, *Orig Life Evol Biosph* **32**(3) (2002) 195
[3] D. Niether *et al.*, *Proc Natl Acad Sci USA* **113**(16) (2016) 4272

Precursers of life



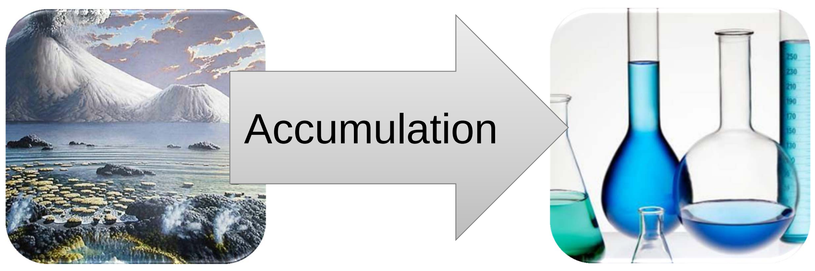
Concentration problem

early earth

low concentrations
ocean ~10^{-7} wt%
shallow lake ~10^{-3} wt%

lab conditions

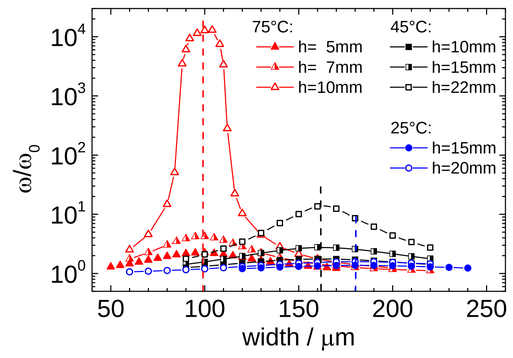
high concentrations
(50 - 100 wt%)

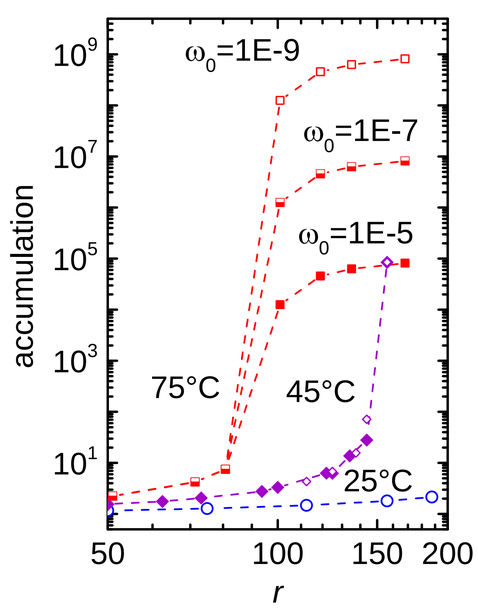


Results

optimal width

- simulations show optimal width L_x for accumulation
- optimal width depends on substance (S_T) and average temperature



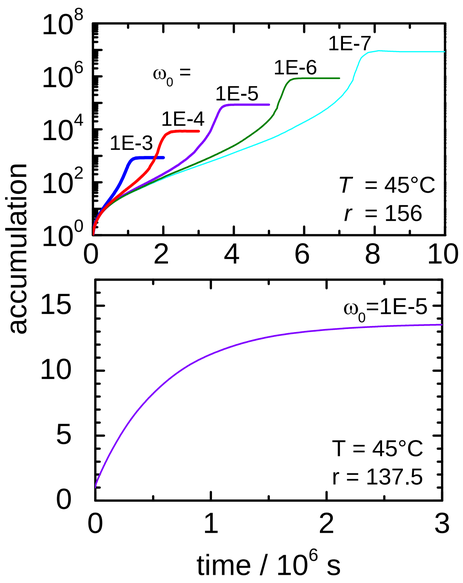


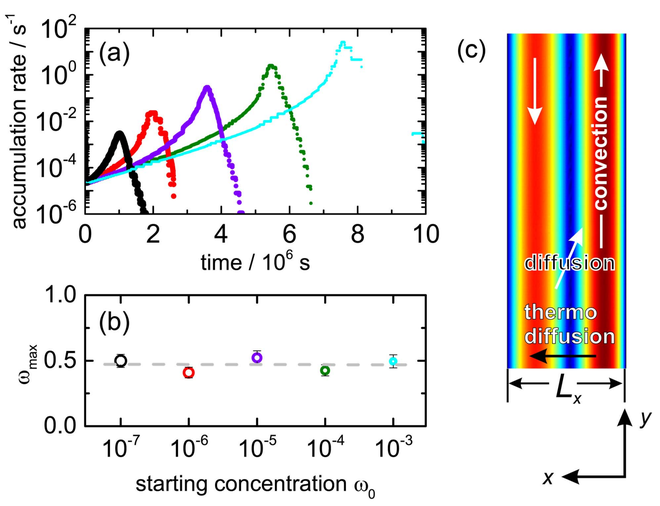
maximum accumulation

- accumulation fold against aspect ratio r with width L_x fixed to optimal value for the respective temperatures
- effective accumulation only if pore is high enough (r has to exceed a certain value)
- at high aspect ratios accumulation saturates independent of starting concentration at formamide concentration of ~ 85 wt%

accumulation rate

- accumulation against time shows similar profiles for different starting concentrations
- lower starting concentrations result in longer times to reach saturation
- for a starting concentration of $\omega_0 = 10^{-5}$ accumulation takes 45 - 90 days
- at low aspect ratios accumulation is ineffective, no rise of accumulation rate





heuristic model

- effective accumulation only if

$$\frac{L_y}{L_x} > \frac{(L_y \cdot v_{conv} + D \cdot \Delta_y \omega) L_x}{4 L_y \cdot \omega(1-\omega) \cdot D_T \cdot \Delta T}$$

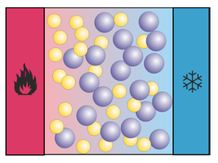
- maximum accumulation rate around $\omega = 0.5$ due to maximum in the term $\omega(1-\omega)$

Thermophoretic accumulation

convection

transport mechanism in gases or liquids
cold, denser material sinks down, hot, lighter material moves up

thermodiffusion



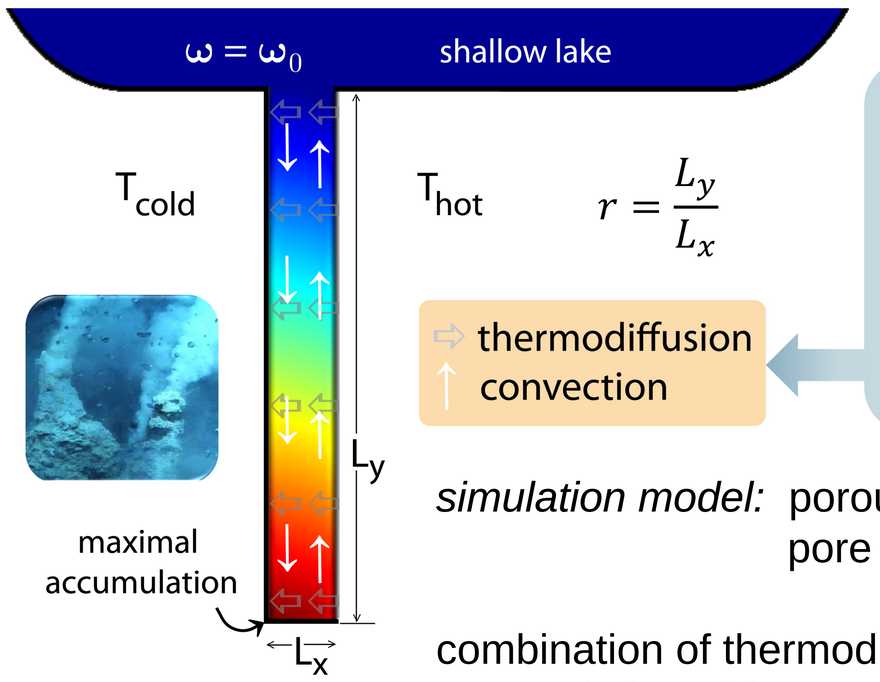
movement of particles driven by temperature gradient

flux $\vec{j}$ is described by

$$\vec{j} = -D\Delta\omega - \omega(1-\omega)D_T\Delta T$$

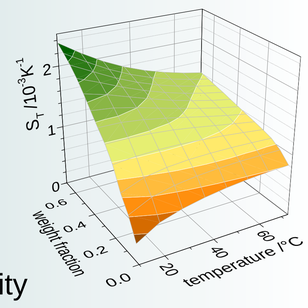
steady state $\vec{j} = 0$

$$S_T \equiv \frac{D_T}{D} = -\frac{1}{\omega(1-\omega)}\frac{\Delta\omega}{\Delta T}$$



thermodiffusion
convection

temperature and concentration dependant parameters of formamide/water:
- Soret coefficient
- density
- viscosity
- heat capacity
- thermal conductivity



simulation model: porous mineral at hydrothermal vents
pore sizes L_x ~ 50 - 200 µm
L_y ~ 1 - 20 mm

combination of thermodiffusion and convection leads to accumulation of formamide in cold bottom corner